

Supporting Information

2-(Arylimino)benzylidene-8-arylimino-5,6,7-trihydroquinoline Cobalt(II) Dichloride Polymerization Catalysts for Polyethylenes with Narrow Polydispersity

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Table S1. Crystal data and structure refinement for **Co2** and **Co5**.

	Co2	Co5
CCDC number	2160864	2160865
Empirical formula	C ₅₈ H ₅₁ Cl ₂ CoN ₃	C ₁₇₂ H ₁₅₀ Cl ₄ Co ₂ N ₆
Formula weight	919.84	2560.63
T (K)	169.99(13)	169.99(13)
Wavelength (Å)	1.54184	1.54184
Crystal system	orthorhombic	monoclinic
Space group	Pbca	P2 ₁ /c
<i>a</i> /Å	10.1343(3)	13.6880(2)
<i>b</i> /Å	16.8486(6)	20.8927(2)
<i>c</i> /Å	59.062(2)	52.9277(7)
α /°	90	90
β /°	90	93.9140(10)
γ /°	90	90
Volume/Å ³	10084.8(6)	15100.9(3)
Z	8	4
ρ_{calc} /cm ³	1.212	1.126
μ /mm ⁻¹	3.938	2.764
F(000)	3848.0	5384.0
Crystal size/mm ³	0.24 × 0.18 × 0.13	0.12 × 0.08 × 0.03
2 Θ range for data collection (°)	5.986 to 151.124	4.548 to 151.076
	-12 ≤ <i>h</i> ≤ 12	-17 ≤ <i>h</i> ≤ 16
Index ranges	-21 ≤ <i>l</i> ≤ 19	-23 ≤ <i>k</i> ≤ 26
	-73 ≤ <i>l</i> ≤ 74	-66 ≤ <i>l</i> ≤ 65
Reflections collected	74898	116664
Independent reflections [R _{int}]	10140(0.0983)	30024(0.0612)
Completeness to θ (%)	99.9	99.8
Goodness of fit on F ²	1.051	1.019
Final R indexes [<i>I</i> ≥ 2 σ (<i>I</i>)]	R ₁ = 0.1428	R ₁ = 0.0636
Final R indexes (all data)	<i>w</i> R ₂ = 0.4052	<i>w</i> R ₂ = 0.1611
	R ₁ = 0.1703	R ₁ = 0.0975
	<i>w</i> R ₂ = 0.4257	<i>w</i> R ₂ = 0.1812
Largest diff peak/hole (e/Å ⁻³)	1.38/-0.65	0.85/-0.50

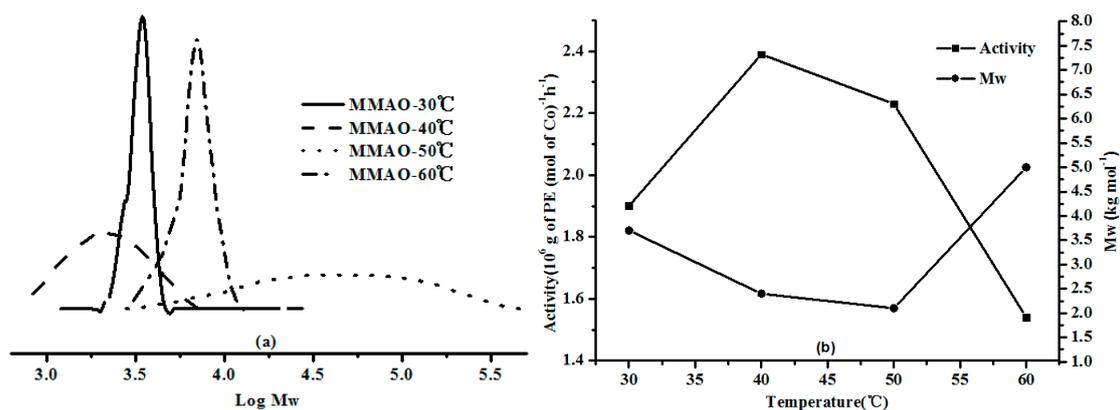


Figure S1. For Co6/MMAO: (a) GPC traces of the polyethylene obtained at different run temperatures and (b) activity and M_w as a function of reaction temperature (entries 1 – 4, Table 4).

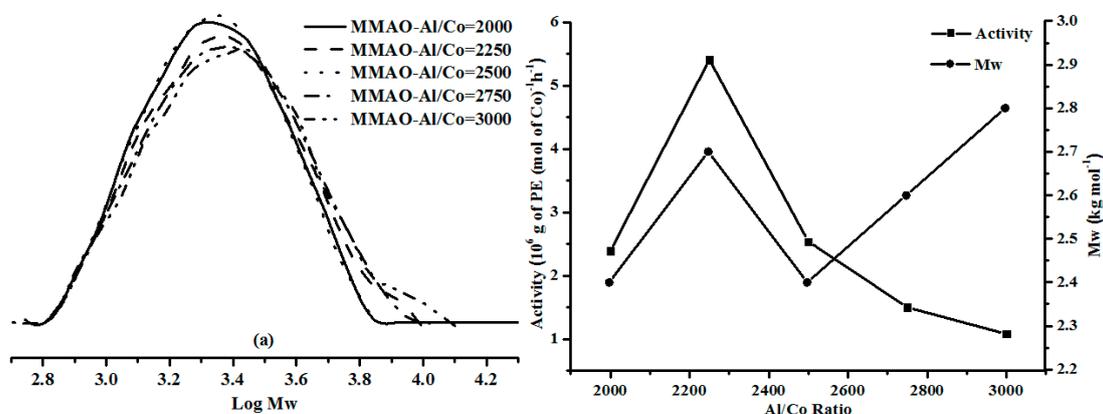


Figure S2. For Co6/MMAO: (a) GPC traces of the polymers obtained at different Al:Co molar ratios and (b) catalytic activity and M_w as a function of Al:Co molar ratio (entries 2, 5 – 8, Table 4).

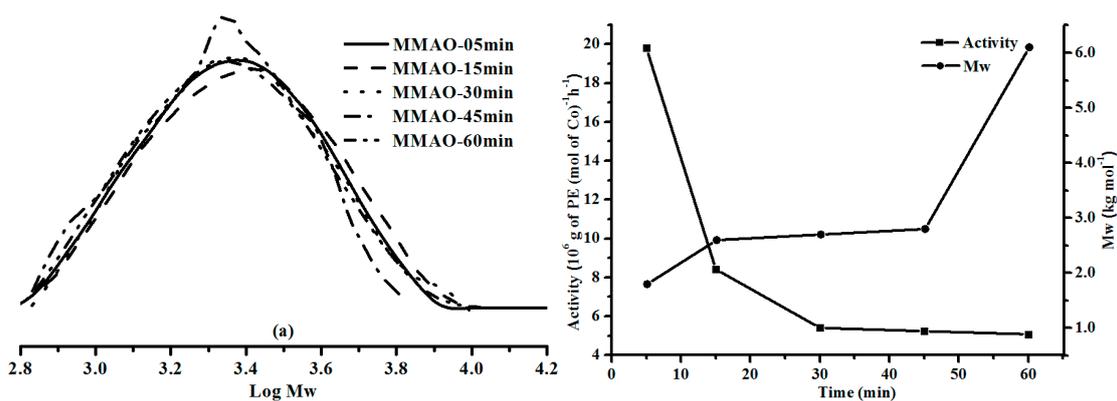


Figure S3. For Co6/MMAO: (a) GPC traces of the polyethylene obtained over the course of time and (b) activity and M_w as a function of reaction time (entries 5, 9 – 12, Table 4).

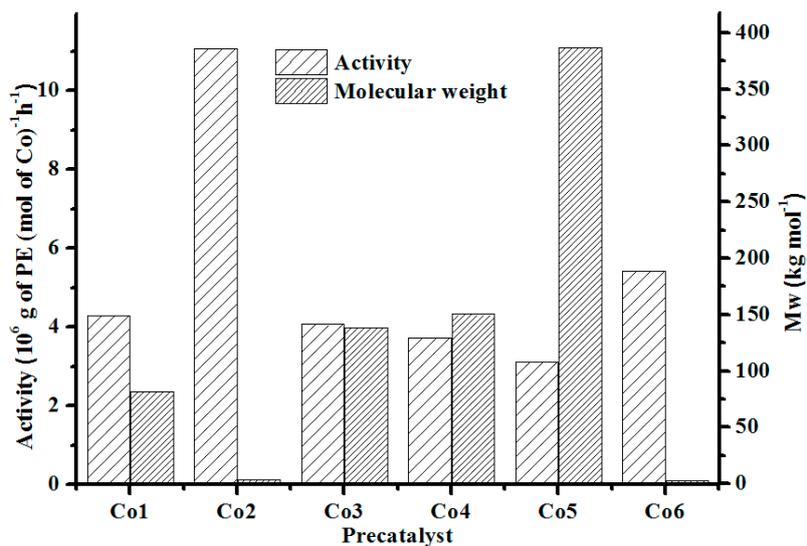


Figure S4. Catalytic activities and molecular weight of the polyethylenes produced by Co1 – Co6; MMAO as co-catalyst in each case (entries 1 – 6, Table 5).

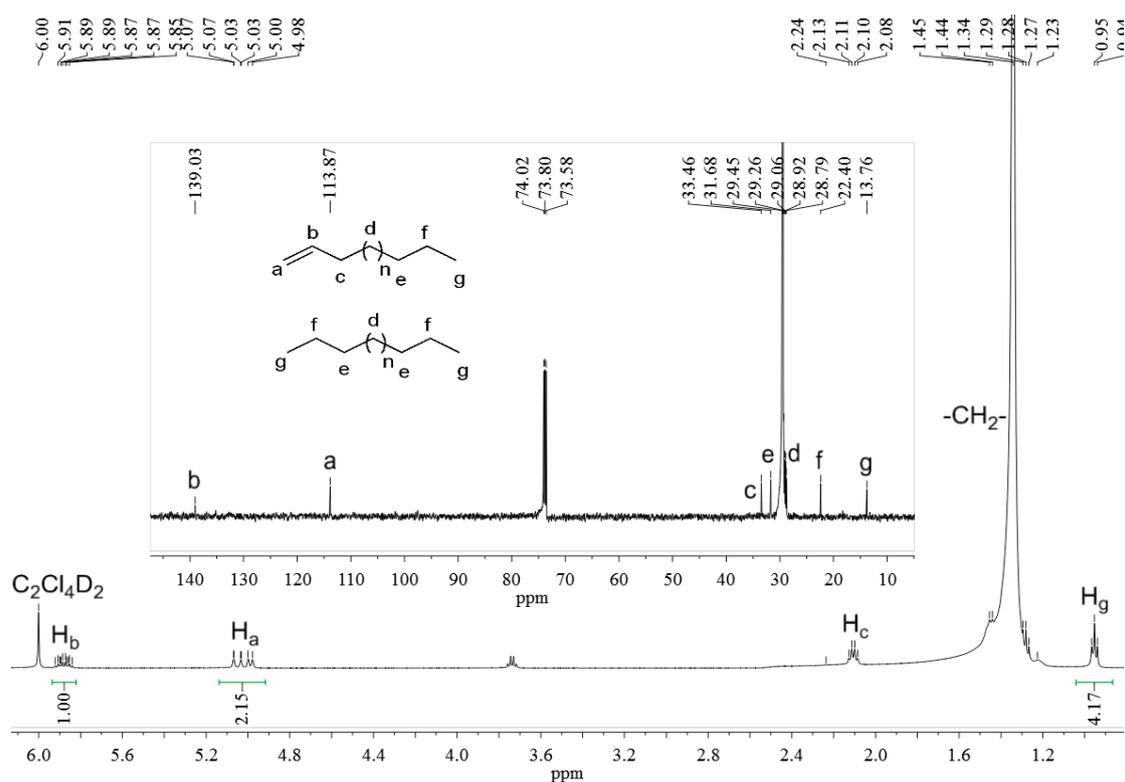


Figure S5. ^1H NMR spectrum of the polyethylene obtained using Co2/MMAO at 40 °C (entry 2, Table 5) along with an inset of the ^{13}C NMR spectrum; both spectra recorded at 100 °C in 1,1,2,2-tetrachloroethane- d_2 .

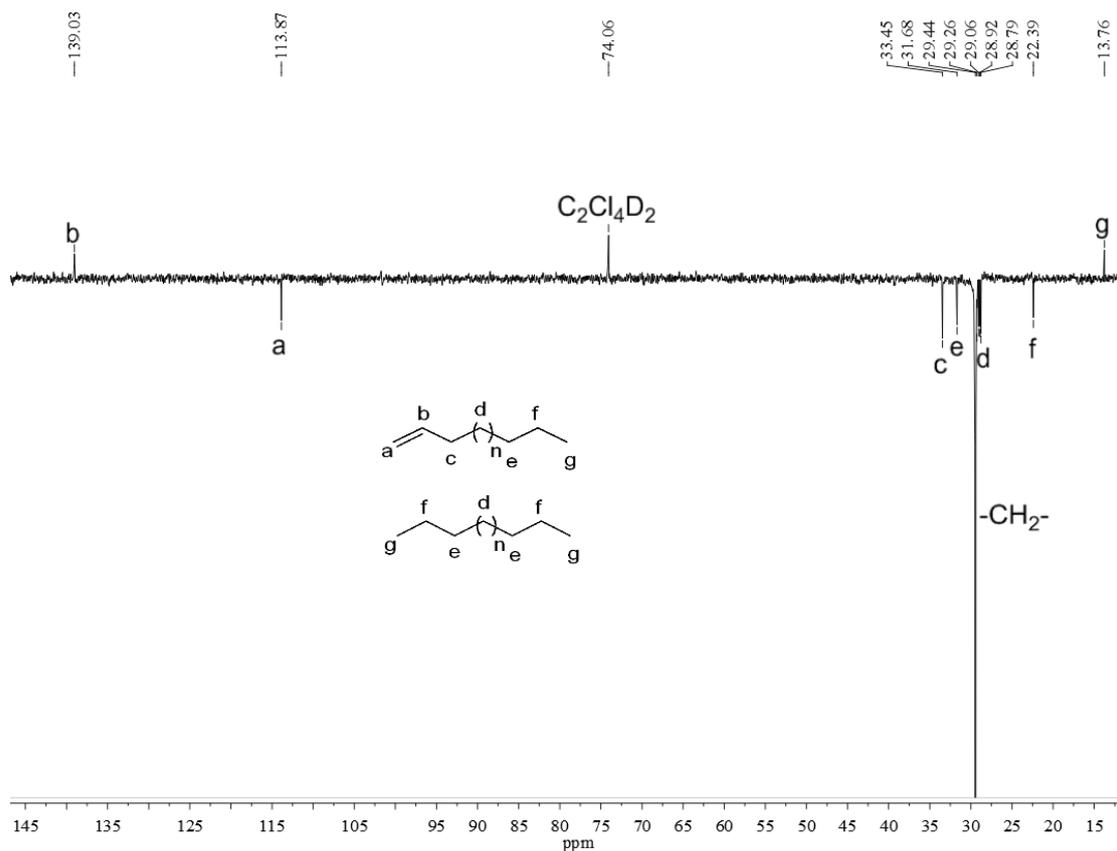


Figure S6. DEPT-135 ^{13}C NMR spectrum of the polyethylene obtained using Co_2/MAO at $50\text{ }^\circ\text{C}$ (entry 2, Table 3).

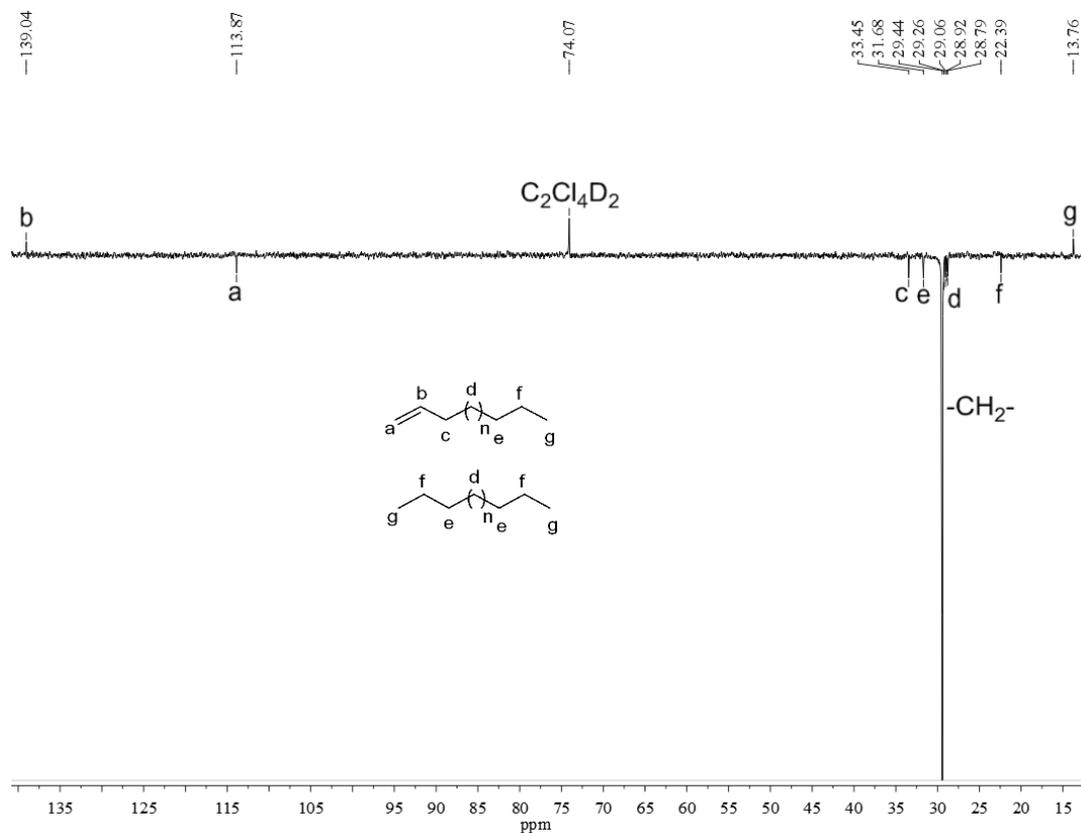


Figure S7. DEPT-135 ^{13}C NMR spectrum of the polyethylene obtained using Co_2/MMAO at $40\text{ }^\circ\text{C}$ (entry 2, Table 5).

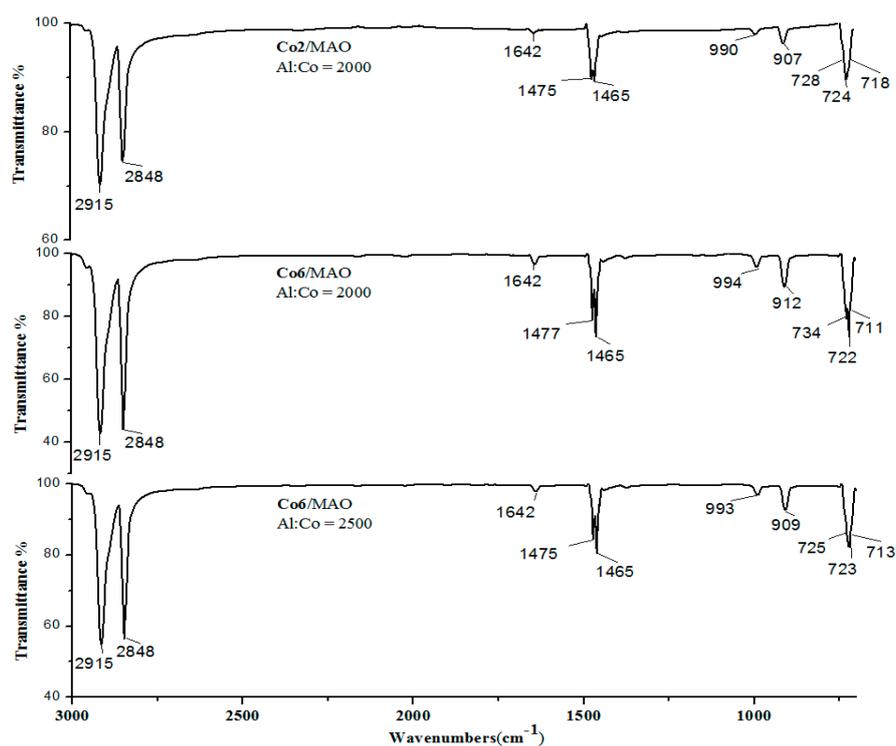


Figure S8. FT-IR spectra of the polyethylene samples generated using Co2/MAO (top, entry 2, Table 3) and Co6/MAO (middle, entry 2, Table 2 and bottom, entry 8, Table 2).

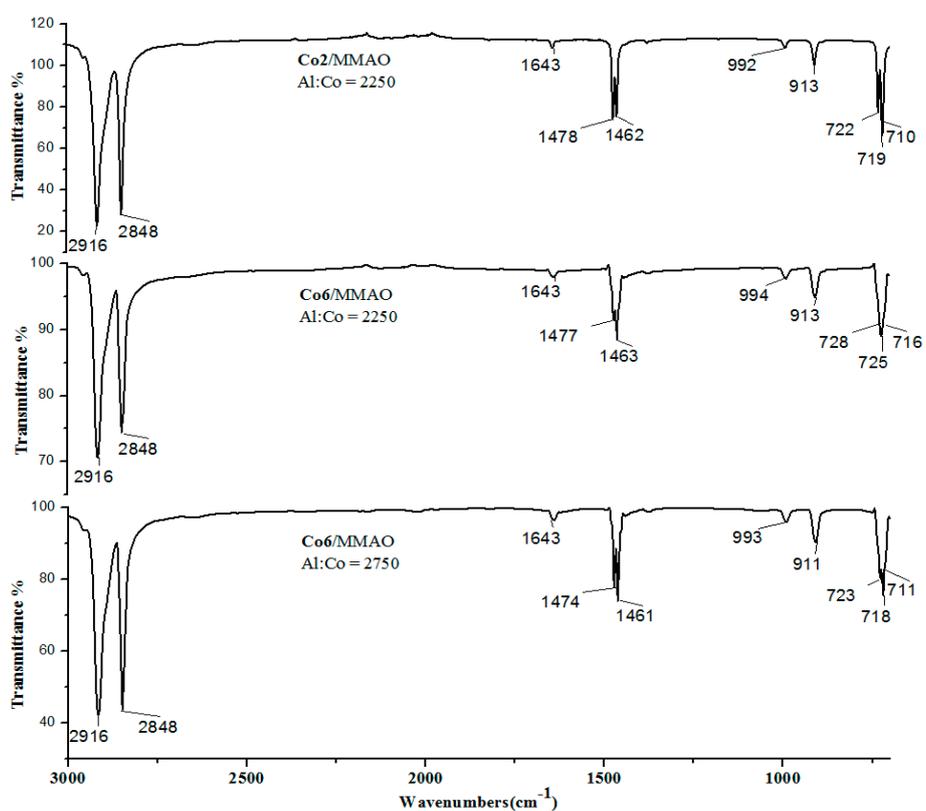


Figure S9. FT-IR spectra of the polyethylene generated using Co2/MMAO (top, entry 2, Table 5) and Co6/MMAO (middle, entry 5, Table 4 and bottom, entry 7, Table 4).